

AD-A277 148



THE DEVELOPMENT OF QUANTUM CHEMISTRY CODES

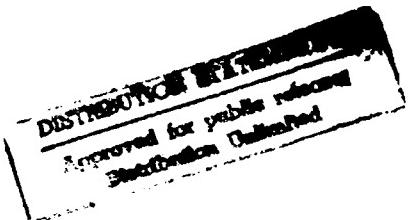
(2)

**Professor N. C. Handy and Dr. R. D. Amos
University Chemical Laboratory
Lensfield Road
Cambridge CB2 1EW
UK**

Grant No. AFOSR-90-0225

**DTIC
ELECTE
MAR 18 1994
S B D**

01 March 1991 - 31 August 1992



DISTRIBUTION STATEMENT A

94-08733



94 3 18* 023

REPORT DOCUMENTATION PAGE			Form Approved OMB No. 0704-0183
<p>Public reporting burden for the collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comments regarding this burden estimate or any other aspect of the collection of information, including suggestions for reducing the burden, to Washington Headquarters Services, Directorate for Information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Paperwork Reduction Project 0704-0183, Washington, DC 20503.</p>			
1. AGENCY USE ONLY (Leave Blank)	2. REPORT DATE	3. REPORT TYPE AND DATES COVERED	
	MAR 1994	SECOND TECHNICAL 01 MAR 91- 31 AUG 92	
4. TITLE AND SUBTITLE		5. FUNDING NUMBERS	
THE DEVELOPMENT OF QUANTUM CHEMISTRY CODES		AFOSR-90-0225	
6. AUTHOR(S)			
PROFESSOR N. C. HANDY DR. R. D. AMOS			
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)		8. PERFORMING ORGANIZATION REPORT NUMBER	
DEPARTMENT OF CHEMISTRY UNIVERSITY OF CAMBRIDGE		DIZ 1009	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)		10. SPONSORING/MONITORING AGENCY REPORT NUMBER	
		EOARD TR-94-C4	
11. SUPPLEMENTARY NOTES			
12a. DISTRIBUTION/AVAILABILITY STATEMENT		12b. DISTRIBUTION CODE	
13. ABSTRACT (Maximum 200 words)			
<p>The Cambridge Analytic Derivatives Package (CADPAC) has continued to be developed as a Computational Chemistry Package, in line with the grant proposal. During the period of this report the following extensions have been made.</p> <ul style="list-style-type: none"> (i) Evaluation of third and fourth derivatives of the SCF energy. (ii) Evaluation of fourth order force constants for MP2 theory. (iii) The development of the theoretical spectroscopy package SPECIRO. 			
14. SUBJECT TERMS		15. NUMBER OF PAGES	
16. PRICE CODE			
17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT

Second Annual Technical Report AFOSR-90-0225

**Professor N. C. Handy, Dr. R. D. Amos
University Chemical Laboratory
Lensfield Road
Cambridge CB2 1EW
UK**

**Full Period of Grant June 1 1990 - August 31 1993
Title of Grant "The Development of Quantum Chemistry Codes"**

Over the entire period of the grant, we have continued to develop our Quantum Chemistry Code, CADPAC.

The specific advances for the period 1 March 1991 - 31 October 1992 are concerned with theoretical spectroscopy.

- (i) The development of a code which calculates analytically the third and fourth derivatives of the Self Consistent Field Energy. This is the first such code.
- (ii) The development of a code which calculates by central finite differences third and fourth order force constants for the correlated Møller-Plesset second order MP2 method.
- (iii) The development of a code, SPECTRO, which accepts the force fields generated in (i) and (ii), and delivers spectroscopic constants such as anharmonic constants, fundamental frequencies and vibration-rotation interaction constants.

Dr. A. Willets, partially funded by this AFOSR grant, have been actively involved with all aspects of this project. Attached is a list of scientific papers which have been published in connection with these developments of CADPAC.

150. SPECTRO - a program for the derivation of spectroscopic constants from provided quartic force fields and cubic dipole fields. J F Gaw, A Willetts, W H Green and N C Handy, Advances in Molecular Vibrations and Collision Dynamics. ed. J M Bowman, JAI, Greenwich CT, 1B,169-185 (1991).

153. Higher Analytic Derivatives. (1) A new implementation for the third derivative of the SCF energy. S M Colwell, D Jayatilaka, P E Maslen, R D Amos and N C Handy. Int J Quant Chem. 40, 179 (1991).

168. Anharmonic Vibrational Properties of CH₂F₂: A comparison of theory and experiment. R.D. Amos, N.C. Handy, W.H. Green, D. Jayatilaka, A. Willetts and P. Palmieri. J.Chem. Phys. 95, 8323 (1991)

174. Higher Analytic Derivatives. (2) The Fourth Derivative of the Self Consistent Field Energy. P. E. Maslen, D. Jayatilaka, S. M. Colwell, R. D. Amos and N. C. Handy. J. Chem. Phys. 95, 7409 (1991)

179. Higher Analytic Derivatives (3) Geometrical Derivatives of the Dipole and Dipole Polarisabilities. D. Jayatilaka, P. E. Maslen, R. D. Amos, and N. C. Handy. Molec. Phys. 75, 271 (1992)

186. Higher Analytic Derivatives IV. Anharmonic Effects in the Benzene Spectrum. P. E. Maslen, N. C. Handy, R. D. Amos and D. Jayatilaka . J. Chem. Phys. 97, 4233 (1992)

Accession For	
NTIS GRA&I	<input checked="" type="checkbox"/>
DTIC TAB	<input type="checkbox"/>
Unannounced	<input type="checkbox"/>
Justification	
per letter	
By	
Distribution	
Availability Codes	
Dist	Avail and/or Special
P	